

d-Proline, n-propoxycarbonyl-. butyl ester

Inchi:	InChI=1S/C13H23NO4/c1-3-5-10-17-12(15)11-7-6-8-14(11)13(16)18-9-4-2/h11H,3-10H2
InchiKey:	SDHRTLAVRSETGE-UHFFFAOYSA-N
Formula:	C13H23NO4
SMILES:	CCCCOC(=O)C1CCCN1C(=O)OCCC
Mol. weight [g/mol]:	257.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.54		Crippen Method
logp	2.341		Crippen Method
mcvol	208.030	ml/mol	McGowan Method
rinpol	1743.00		NIST Webbook
rinpol	1743.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320820&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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